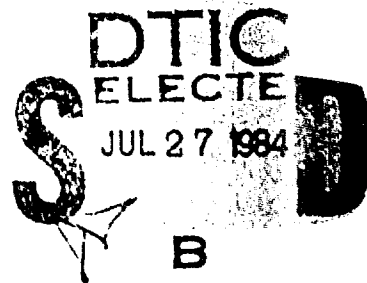DISTRIBUTIONS OF CENTRAL QUADRATIC FORMS

IN NORMAL VARIABLES:

A COMPARISON OF ALGORITHMS

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Quadratic functions of multivariate normal random variables arise with surprising frequency in certain social science theories. However, they seem to be rarely used in applications because of the numerical difficulties in computing their distribution functions. This thesis implements a new strategy for computing the distribution function for an arbitrary positive definite quadratic form in multivariate normal variables. Alternative algorithms are reviewed. Comparison trials are reported to show that the new algorithm is at least a accurate and reliable as the alternative algorithms.

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1. INTRODUCTION

A random variable Y is a quadratic function of n independent, multivariate normal variables if for some positive definite matrix A and vector b, Y has the same distribution function as

$$(Z - b)^T A(Z - b)$$

where

$$Z^T = <Z_1, Z_2, \ldots, Z_n>$$

is a vector of independent standard normal variables. This thesis is restricted to the important "homogeneous" special case in which b is zero. Without a loss of generality, A can be taken to be a diagonal matrix since for some orthonormal matrix U,

$$Z^T A Z = (ZU)U^T AU(ZU)^T$$

and ZU is "multinormal" whenever Z is. Thus this thesis is concerned with a variable of the form

(1) $$Y = \sum_1^n \alpha_i Z_i^2,$$

where the Z_i are independent, multivariate normal and the α_i are positive constants.

The distribution function of such variables has numerous applications. Johnson and Kotz (1970, Chapter 29, Sec. 10) list engineering applications. Levine (1983, 1984 - Proceeding of the Computerized Adaptive Testing Conference, David

Weiss, Editor) argues that such variables are important because they enable one to test the hypothesis that a multiple choice test item is equally hard for two ethnic groups. In addition he shows that such variables can be used to decide if a test item's properties have been affected by changes in educational practices or unauthorized use of the item. Finally, Levine (1984) proposes using such variables to statistically test the fundamental assumption of modern test theory, "local independence."

It is impractical to publish tables for these variables because the shapes of distribution function depend in a complicated way on the numbers α_i. Therefore, a numerical algorithm is needed to approximate the distribution function

$$F(y;\alpha_1,\alpha_2,\ldots,\alpha_n) = Prob(Y \leq y).$$

A satisfactory algorithm must be accurate and numerically stable for values of y and α_i that occur in actual social science applications.

The major published algorithms for computing F involve the "series expansions" of the distribution function, i.e., representations of the form

$$F(y) = \sum_{k=0}^{\infty} a_k g_k(y).$$

where $\{g_k(y)\}$ is a sequence of known functions of y and a_k is a coefficient of $g_k(y)$ which does not depend on y.

This thesis begins with a discussion of series expansion algorithms. It will be demonstrated that the series expansion algorithms fail in some important cases. Our alternative algorithm (DLT-algorithm) is then described, programmed, and evaluated.

2. SERIES EXPANSIONS

Johnson and Kotz (1970) obtain a unified treatment of the various series expansions by analyzing the derivative or "density" of F. To do this, they specified functions $h_k(y)$ and obtained coefficients a_k so that the expansion

$$f_N(y) = \sum_{k=0}^{N} a_k h_k(y)$$

converges to the density $f(y)$. A sequence of approximations {F_N} of the distribution function can then be obtained by integrating the $f_N(y)$. Thus,

$$(2) \quad F_N(y) = \sum_{k=0}^{N} a_k g_k(y),$$

where $g_k(y)$ is obtained by integrating $h_k(y)$. Their method of obtaining the a_k is presented in Kotz, Johnson, and Boyd (1967) and is briefly summarized in the Appendix.

Three forms of $F_N(y)$ for central quadratic variables are tested here. These forms, the power series, Chi-square series, and the Laguerre series, are presented in Kotz, et al (1967) and displayed here as equations (3) - (9). In the power series, $g_k(y)$ is a power of y. In the Chi-square series, $g_k(y)$ is a χ^2 distribution function with degrees of freedom which depends on k. Finally, in the Laguerre series, $g_k(y)$ is obtained from the Laguerre polynomial with degree k, presented in equation (9).

2.2 χ^2 S series equations

The equation

(5) $$F_N(y) = \sum_{k=0}^{N} c_k \, G(n + 2k; \, y/\beta)$$

also converges to $F(y)$. Here, 1) $G(n + 2k; \, y/\beta)$ is the χ^2 distribution of y/β at $n+2k$ degrees of freedom; 2) the c_k are obtained recursively by

(6) $$c_0 = \prod_{j=1}^{n} (\beta/\alpha_j)$$

$$c_k = \frac{1}{2k} \sum_{r=0}^{k-1} c_r \sum_{j=1}^{n} [1 - \beta/\alpha_j]^{k-r} \; ;$$

and 3) β is a number which makes

$$\epsilon = \max_j |1 - \beta/\alpha_j|$$

as small as possible, which Ruben (1962) claimed to be near $\beta^* = 2\alpha_1\alpha_n/(\alpha_1 + \alpha_n)$. Also, the expression

$$E_N(y) = \prod_{j=1}^{n} (\frac{\beta}{\alpha_j})^{1/2} \frac{\Gamma(n/2+N+1)}{\Gamma(n/2)} \frac{\epsilon^{N-1}}{(N+1)!} (1-\epsilon)^{-n/2-N-1} G_N(\cdot),$$

where $G_N(\epsilon) = G[n+2N+2; \, (1-\epsilon)y/\beta]$, is an upper bound of the error of approximation when $\epsilon < 1$, which holds for $\beta = \beta^*$ whenever $\alpha_1 < 1$ (as was the case for all applications reported here).

After the series expansions are presented (along with equations for the error bounds), algorithms for computing these expansions are developed. Convergence and stability of these algorithms were tested for data arising in applications (Tables 1 and 2). Tables 2 through 5 show the values of $F_N(y)$, along with the rate of convergence and the error bounds at various values of N.

2.1 Power series equations

The following series converges to $F(y)$:

(3) $$F_N(y) = (\frac{y}{2})^{n/2} \sum_{k=0}^{N} \frac{c_k(-1)^k(y/2)^k}{\Gamma(n/2 + k + 1)} ,$$

where n is the number of terms in $y = \sum_{i=1}^{n} \alpha_i Z_i^2$ and c_k is obtained by the following recursive formulas:

(4) $$c_0 = \prod_{j=1}^{n} \alpha_j^{-1/2}$$

$$c_k = \frac{1}{2k} \sum_{r=0}^{k-1} c_r \sum_{j=1}^{n} \alpha_j^{-(k-r)} .$$

Also, the difference between $F_N(y)$ and the actual $F(y)$ is bounded by

$$E_N(y) = \frac{(\frac{y}{2})^{n/2+N+1}}{\Gamma(n/2+N+2)} c_{N+1} ,$$

which decreases with N .

2.3 Laguerre series equations

The series

$$F_N(y;\underline{\alpha}) = G(n;y/\beta) +$$

(7)
$$\sum_{k=1}^{N} c_k \frac{(k-1)!}{\Gamma(\frac{n}{2}+k)} \left(\frac{y}{2\beta}\right)^{n/2} e^{-\frac{y}{2\beta}} L_{k-1}^{(\frac{n}{2})}\left(\frac{y}{2\beta}\right)$$

converges to $F(y)$. Here,

$$c_o = 1$$

(8)
$$c_k = \frac{1}{2k} \sum_{r=0}^{k-1} c_r \sum_{j=1}^{n} (1-\alpha_j/\beta)^{k-r}.$$

Also, the term $L_{k-1}^{(n/2)}(x)$ is the generaliz.d Laguerre polynomial defined by Rodrigues' formula

(9)
$$L_{k-1}^{(\frac{n}{2})}(x) = \frac{1}{(k-1)!} e^x x^{-\frac{n}{2}} \frac{d^{k-1}}{du^{k-1}} e^{-u} u^{k-1+\frac{n}{2}}\Big|_{u=x}$$

Finally, β minimizes $\epsilon = \max_j |1-\alpha_j/\beta|$ and (unlike the χ^2 series representation) may depend on the α_j (for $\alpha_j \equiv 1$, $\beta=1/2(\alpha_1+\alpha_n)$) makes $\epsilon=0$ and $c_k=0$ for $k\geq 1$). The equation

$$E_N(y) = \frac{n}{N+1} g(n+2;\frac{y}{\beta}) e^{y/4\beta} \frac{(\sqrt{\epsilon})^{N+2}}{(1-\sqrt{\epsilon})^{n/2+2}}$$

provides an error bound for the Laguerre series.

2.4 Description of the algorithms

The computing algorithms necessary to obtain approximations using equations (3) - (9) are not always easy to write. One problem is that a term can be represented as the product of two extreme values. For example, in equation (3), c_k increases without bound when α_j is very small whereas $(y/2)^k/\Gamma(n/2 + k + 1)$ decreases to zero for small y. The result is generally a product which is moderate in value. However, the product of extreme values may be subject to round-off error, producing an erroneous approximation to the distribution. Some ingenuity is required to keep intermediate results within bounds.

The following algorithms attempt to keep roundoff error to a minimum. The series equations are rewritten in a way which can easily be translated to computer code. Whenever necessary the code which evaluates each term in the series is presented. The required number of computations is also provided. The algorithms for the power series, χ^2 series, and the Laguerre series are now discussed in that order.

Power series

Equation (3) can be expressed as

$$F_N(y) = \sum_{k=0}^{N} c_k' ,$$

where

(10)
$$c_k' = \frac{c_k (\frac{y}{2})^{\frac{n}{2}} (-\frac{y}{2})^k}{\Gamma(\frac{n}{2} + k + 1)} .$$

Substitution of (4) into (10) gives

$$c_k' = \frac{1}{2k} \sum_{r=0}^{k-1} c_r \sum_{i=1}^{n} \alpha_i^{-(k-r)} (\tfrac{y}{2})^{n/2} \frac{(-\tfrac{y}{2})^k}{\Gamma(\tfrac{n}{2} + k + 1)}$$

$$= \frac{1}{2k} \sum_{i=1}^{n} \sum_{r=0}^{k-1} \frac{c_r' \alpha_i^{-(k-r)}(-\tfrac{y}{2})^{k-r}}{(\tfrac{n}{2}+k)\ldots(\tfrac{n}{2}+r+1)},$$

which can be computed by the following modification of Horner's method:

$$c_0' = \frac{\prod_{j=1}^{n} (\alpha_j^{-1/2}) (\tfrac{y}{2})^{\frac{n}{2}}}{\Gamma(\tfrac{n}{2} + 1)}$$

```
     DO 30 k=1, N
     sum=0
     DO 20 i=1, n
     p=c_0' * (-y/2)/(n/2 + 1)

     DO 10 r=1, k-1
     p=(p/α_i + c_r') * (-y/2)
            ─────────────
             n/2 + 1 + r

10   CONTINUE
     sum=sum+p/α_i
20   CONTINUE
     c_k' = sum/2k
30   CONTINUE
```

Intermediate results tend not to be extreme with this algorithm.

The number of computations required in the power series algorithm can be derived as follows. The c_0' term requires 1) n-1 multiplications, n divisions $(1/\alpha_i)$, and n computations of the square root to obtain

$$c_0 = \prod_{j=1}^{n} \alpha_j^{-1/2} ;$$

2) $\frac{n}{2} - 1$ multiplications to obtain $(\tfrac{y}{2})^{n/2}$ if n is even, and n/2 multiplications if n is odd, or an average of (n-1)/2 multiplications; 3) $\frac{n}{2} - 1$ divisions and additions to obtain

$$\frac{(\tfrac{y}{2})^{\frac{n}{2}}}{\Gamma(\tfrac{n}{2}+1)}$$

if n is even, and $\frac{n}{2}$ divisions, $\frac{n}{2} - 1$ additions, and one square root evaluation if n is odd, or an average of n - 1 computations; and 4) one multiplication of the values obtained in 1) and 3) to obtain c_0', or a total of $\frac{9}{2}n - \frac{3}{2}$ computations. Each c_k' term $(k \geq 1)$ requires 1) 2k divisions, k multiplications, and 2k additions for each of n iterations within the i-loop and 2) one multiplication and division (by 2k) to obtain c_k', or 5nk + 2 computations. The calculation of all the c_k' thus requires $(\frac{9}{2}n - \frac{3}{2}) + (\frac{5}{2}n N(N+1) + 2N)$ computations. Finally, N further additions of the c_k' terms are required to obtain $F_N(y)$, giving a total of $\frac{9}{2}n + \frac{5}{2}nN^2 + (\frac{5}{2}n+3)N - \frac{3}{2}$ computations.

plications. Then a subtraction is performed to obtain each $1-\beta/\alpha_j$ term. Finally, for each c_k ($k>1$) term, nk multiplications and nk additions are required through the i-loop and one multiplication and division by 2k are required to obtain c_k . Thus, all the c_k terms require $3n-1+3nN+3nN^2$ computations.

The distribution function $G(n+2k;y/\beta)$ was calculated from the following series (Abramowitz & Stegun, 1965). For odd ν ,

$$1 - G(\nu;x^2) = 2[1-\Phi(x)] + \left(\frac{2}{\pi}\right)^{1/2} e^{-x^2/2} \sum_{r=1}^{\frac{\nu-1}{2}} \frac{x^{2r-1}}{1\cdot3\cdot5\cdots(2r-1)} ,$$

where $\Phi(x)$ is the standard normal distribution function. The value of $G(\nu;y)$ can then be computed from the following algorithm:

```
        term=y^1/2
        sum=term
        xn=1
        DO 50  i=2, (ν-1)/2
           xn = xn + 2
           term=term * (y/xn)
           sum = sum + term
50      CONTINUE
        sum = 2*[1-Φ(y^1/2)]+(2/π)^1/2*e^-y/2*sum
        G(ν;y)=1-sum
```

An application of this algorithm for $G(n+2k;y/\beta)$ requires 1) one initial evaluation of the square root of y/β and one division of $n+2k-1$ by 2 ; 2) two additions, one multiplication, and one division for each iteration within the i-loop, or $2(n-1) + 4k - 1$ computations through the loop; and 3) two divisions, three multiplications, two subtractions, one addi-

---

Chi-square series

Unlike the power series, the factors of each term in the χ^2 series expansion (5) , c_k and $G(n+2k;y/\beta)$, were computed separately before being applied to (5) . This is because both factors decrease or remain steady with k . Equation (6) shows this to be true for c_k , since

$$|c_k| \leq \frac{n}{2k} \sum_{r=0}^{k-1} |c_r| \epsilon^{k-r} ,$$

and β/α_j and thus ϵ are less than 1 whenever $\alpha_j < 1$ (as was the case for all data analyzed here). Also, the G functions decrease with k for constant y/β , since the variance of a χ^2 distribution increases with its degrees of freedom.

The c_k can be calculated according to (6) using the following modification of Horner's method:

```
        DO 20 k=1, N
           sum=0
           DO 10  i=1, n
              p=c_o
              DO 5  r=1, k-1
                 p=p*[1-B/α_j] + c_r
5             CONTINUE
              sum=sum + [1-B/α_j] * p
10         CONTINUE
           c_k = sum/2k
20      CONTINUE
```

The number of calculations can be determined as follows.

First, $c_o = \sum_{i=1}^{n} (\beta/\alpha_i)$ requires n divisions and $n-1$ multi-

$$\frac{\Gamma(\frac{n}{2} + N + 1)}{\Gamma(\frac{n}{2})\,(N + 1)!} \cdot \frac{\epsilon^{N+1}}{(1-\epsilon)^{n/2+N+1}} \quad .$$

may increase with N and must then be offset by the decreasing
G(n+2N+2;(1-ε)y/β) .

The Wilson and Hilferty (1931) cube root approximation
$(\chi^2/\nu)^{1/3} \sim N(1-\frac{2}{9\nu}, \frac{2}{9\nu})$ approaches zero much faster than either the
χ^2 distribution approximation or the $N(\nu, 2\nu)$ approximation,
and so was used whenever the degrees of freedom exceeds 100 .
This requires 1) one multiplication and one division to compute
2/9ν ; 2) three divisions, two subtractions, one square root
computation, and one cube root computation for the cube root
approximation; and 3) a computation of the standard normal
distribution of the above approximation, or a total of 10
computations.

The evaluation of the χ^2 series thus requires
1) $3n + nN^2 + 3nN - 1$ computations for the c_k terms;
2) an average of $2n(N+1) + 2(N+1)(N+2) + 6$ computations in
approximating the χ^2 distribution function if N is small
or about 10N computations for the normal distribution function
of the cube root approximation if N is large; and 3) N+1
multiplications and N additions in summing the $c_k \cdot G(n+2;\ldots)$
terms. The total number of computations is related to nN^2 ,
as opposed to $\frac{5}{2}nN^2$ for the power series.

tion, one square root evaluation, one exponentiation, and one
evaluation of the standard normal distribution to obtain the
distribution function, or a total of 2n + 4k + 10 computations.

For even ν ,

$$1 - G(\nu; x^2) = e^{-x^2/2}\left[1 + \sum_{r=1}^{\frac{\nu-2}{2}} \frac{x^{2r}}{2\cdot4\cdot6\cdots(2r)}\right] .$$

The distribution function G(ν;y) can then be computed according to the algorithm

```
      xn=0
      sum=1
      term=1
      DO 50 i=1, (ν-2)/2
      xn=xn + 2
      term=term * (y/xn)
      sum=sum + term
50    CONTINUE
      G(ν;y) = 1 - e^{-y/2} * sum
```

An application of this algorithm for G(n+2k;y/β) requires
1) one subtraction and one division to obtain (n+2k-2)/2 ;
2) two additions, one multiplication, and one division for each
iteration within the i-loop, or 2(n-2) + 4k computations
through the loop; and 3) one division, one multiplication,
one subtraction, and one exponentiation to obtain the distri-
bution function, or a total of 2n+4k+2 computations.

However, the previous algorithm for calculating the
χ^2 distribution is not accurate when the degrees of freedom
exceeds 100. Furthermore, the usual normal approximation
$\chi^2_\nu \sim N(\nu, 2\nu)$ is very poor at the tails. A better approximation
is necessary, especially for the error bound, where the factor
which depends on N ,

let

$$g_0(x) = \frac{e^{-x} x^{n/2}}{\Gamma(\frac{n}{2}+1)}$$

and

$$g_1(x) = \frac{x}{\frac{n}{2}+1} g_0(x).$$

Then the derivative of $g_1(x)$ is

$$g_1'(x) = \frac{d}{dx} \frac{e^{-x}x^{n/2+1}}{\Gamma(\frac{n}{2}+2)}$$

$$= g_0(x) - g_1(x).$$

Similarly, if

$$g_k(x) = \frac{x}{\frac{n}{2}+k} g_{k-1}(x)$$

then

$$g_k'(x) = g_{k-1}(x) - g_k(x)$$

and

$$g_k^{(k)}(x) = g_{k-1}^{(k-1)}(x) - g_k^{(k-1)}(x).$$

Equation (11) is then just $g_{k-1}^{(k-1)}(y/2\beta)$.

The evaluation of the kth derivative of $g_{k-1}(x)$ thus requires 1) the k-1 derivatives of $g_{k-1}(x)$ and 2) the

Laguerre series

Equation (7) reduces to the following equation:

$$F_N(y) = G(n;y/\beta) + \sum_{k=1}^{N} \frac{c_k}{\Gamma(\frac{n}{2}+k)} \frac{d^{k-1}}{dx^{k-1}} e^{-x} x^{n/2+k-1}\Big|_{x=y/2\beta}$$

First, the c_k were calculated separately by an algorithm similar to that for the χ^2 series. The c_k in (8) do not grow too large, since α_j/β ranges between $2/[1+\alpha_1/\alpha_n]$ and $2/[1+\alpha_n/\alpha_1]$ for $\beta=\frac{1}{2}(\alpha_1+\alpha_n)$. Also, comparison of equations (6) and (8) shows that the c_k for the two series differ only in that 1) $c_0=1$ *for the Laguerre series and* 2) c_k *for the Laguerre series depends on powers of* $1-\alpha_j/\beta$, whereas that for the χ^2 series depends on powers of $1-\beta/\alpha_j$, so it can be argued that the evaluation of all the c_k requires $2n + 3nN + nN^2$ computations.

Second, $G(n;y/\beta)$ was evaluated using the χ^2 distribution algorithm discussed previously. This requires on the average $2n+6$ computations.

Finally, the term

(11) $$\frac{1}{\Gamma(\frac{n}{2}+k)} \frac{d^{k-1}}{dx^{k-1}} e^{-x} x^{n/2+k-1}\Big|_{x=y/2\beta}$$

can be evaluated by the following recursive algorithm. First

(k-1)st derivative of $g_k(x)$. The former are stored in a separate vector and can be replaced by the k derivatives of $g_k(x)$ as they are calculated.

The computations required for the $g_k^{(k)}(x)$ can be broken down into the following. First, the calculation of $g_0(x)$ requires 1) one exponentiation and one division (by e^x) and 2) n/2 - 1 additions, multiplications, and divisions if n is even, or n/2 - 1 additions, n/2 multiplications and divisions, and one square root evaluation if n is odd, or a total of $\frac{3}{2}n + \frac{1}{2}$ computations. Next, given the k-1 derivatives of $g_{k-1}(x)$, the calculation of $g_k^{(k)}(x)$ requires 1) one addition, multiplication, and division in the calculation of

$$g_k(x) = \frac{x}{\frac{n}{2}+k} g_{k-1}(x)$$

and 2) k subtractions in the calculations of the k derivatives of $g_k(x)$, or a total of k+3 computations. Thus, the total number of computations required for $g_0(x)$ and the N-1 $g_k^{(k)}(x)$ terms is $\frac{3}{2}n + \frac{N(N-1)}{2} + 3(N-1) + \frac{1}{2}$ on the average.

The Laguerre series approximation can then be calculated from the equation

$$F_N(y) = G(n;y/\beta) + \sum_{k=1}^{N} c_k g_{k-1}^{(k-1)}(y/2\beta) .$$

This requires: 1) $2n + 3nN + N^2$ computations for the c_k terms; 2) 2n+6 computations on the average for $G(n;y/\beta)$;

3) $\frac{3}{2}n + N^2/2 + \frac{5}{2}N - \frac{5}{2}$ computations for the $g_k^{(k)}(x)$ terms; and 4) N additions and N multiplications in combining the previous terms, or a total of $\frac{11}{2}n + (n+\frac{1}{2})N^2 + (3n+\frac{9}{2})N + \frac{7}{2}$ computations on the average. The dominating term, $(n+\frac{1}{2})N^2$, is smaller than that for either power series $(\frac{5}{2}nN^2)$ or the χ^2 series $[(n+2)N^2]$.

2.5 Testing the algorithms

The above algorithms were applied to testing the difference between pairs of curves obtained in item response theory. These curves relate the probability of an item response to a latent ability trait, and can be derived from response data by various methods (e.g., Lord, 1980). In one application, the sum of squared difference between such an item response curve and a particular three-parameter logistic curve was reduced to the form given by (1) by a method described in Levine (1984). In a second application, Levine (1983) obtained such a form for the sum of squared difference between response curves of an item given to two populations.

Sets of values of α_1, α_2, α_3, and

$$y = \sum_{i=1}^{3} \alpha_i Z_i^2$$

and

obtained from the two applications are presented in Tables 1 and 2 The first four sets pertain to the first application and the last two sets pertain to the item bias application. Sets 1 and 2 are based on responses to an 85 - item Scholastic

Aptitude Test; sets 3 and 4 are based on responses to a 35 - item Armed Services Vocational Aptitude Battery (ASVAB), Form 8A, Word Knowledge; and sets 5 and 6 are based on responses to the Metropolitan Achievement Test, Form F, Reading Comprehension.

Convergence

Table 2 shows the approximation $F_N(y)$ obtained by the power series, χ^2 series, and the Laguerre series algorithms at N=200 (the value of y corresponding to each set is shown in the second column). This value is correct in at least four decimal places for all sets except set 1. Here, the power series converges to a value way outside the acceptable [0,1] , and the Laguerre series approximation is correct at only two decimal places when N is 200 and breaks down at a larger N before converging.

Set 1 can be distinguished from the other sets in that both of the following conditions are true. First, the value of F is relatively high (~.93644 obtained by other methods). Second, the ratio of variances α_1/α_n , which Gideon and Gurland (1976) calls the spread factor, is also relatively high (.35).

These two conditions alone do not always affect accuracy, since sets 3 and 4 are characterized by a very high spread factor (>70 , as indicated in the last column of Table 1) and sets 2 and 5 induce F values greater than .97 . However, when the value in one condition is high, there is good reason to believe that increasing the value in the other

Table 1

Quadratic Form α- Weights

Set ID	α_1	α_2	α_3	α_1/α_3
1	.023707	.0028379	.00067261	35.246
2	.043270	.0084118	.0044516	9.720
3	.036190	.012882	.00049934	72.476
4	.075770	.023986	.0010011	75.686
5	.0015294	.0074991	.00067151	2.276
6	.032791	.0061423	.0013066	25.096

condition will deleteriously affect convergence. For example, increasing y from .0026888 to .26888 in set 3 ($\alpha_1/\alpha_n \sim 72$) results in a breakdown of both the power serie and the Laguerre series algorithms. Also, the addition of $\alpha_4 = .0000697$ to all sets, which increases the spread factor, degrades the performance of all three algorithms.

The two conditions of high spread factor and high F can individually affect speed of convergence. Table 3 shows the N required for convergence at five decimal places. First, note that convergence of the power series is slower for set 5, which induces an F value near 1.0. Also, note that convergence of the Laguerre series is slower for sets 3 and 4, which are characterized by high spread factors (see Figure 1, which compares the Laguerre series with the 1st order difference algorithm discussed later). Finally, although the χ^2 series converges to the correct value for set 1, the required N is larger than that for the other sets.

The cause of nonconvergence or slow convergence may depend on the algorithm. For the power series, a breakdown may result from extreme values of the partial sums which induce roundoff error. Since $c_k > 0$ for all k due to positive α_i in equation (4), the c_k' term in (10) is alternately positive and negative, so the F_N fluctuate about the true value F. These fluctuations can be large before convergence when α_i is small, as in set 6 (see Table 4), in which F_N does not even fall within acceptable bounds until N=41. Roundoff error generally occurs when the partial sums are astronomical (e.g., $\pm 10^{24}$ for set 1).

Table 2

F_{200} Determined by Series Methods[1]

Set	y	Power Series	χ^2 series	Laguerre series[2]
1	.085373	_[3]	.93644355	.92917662
2	.23052	.97458525	.97459032	.97459032
3	.0026888	.04955647	.04955647	.04955538
4	.020667	.20233724	.20233724	.20233253
5	.035680	.99998839	.99999735	.99999735
6	.048292	.72613215	.72613215	.72613215

[1] n=3

[2] B=($\alpha_1 + \alpha_3$)/2

[3] outside the interval [0,1]

Figure 1

Table 3

N Required For Convergence Of Series[1]

Set	Approximation		
	Power series	χ^2 series	Laguerre series[2]
1	-[3]	49	-[4]
2	11	23	26
3	11	8	219
4	3C	15	221
5	77[5]	13	3
6	53	21	66

[1]Agreement with the correct value at 5 decimal places

[2]$_\beta = (\alpha_1 + \alpha_3)/2$

[3]Does not converge to value within [0,1]

[4]Does not converge at all

[5]Does not converge to correct value at 5 decimal places

For the Laguerre series, the fluctuations of the partial sums about F are smaller (see Figure 1 for the set 4), and so they may merely affect speed of convergence. The breakdown seems to occur for set 1 because the $g_{k-1}^{(k-1)}$ grow large, perhaps from roundoff error of the differences calculated to obtain them, while the c_k decrease with k (the $g_{k-1}^{(k-1)}$ and c_k, however, are generally not as extreme as the corresponding terms in (10) for the power series).

The slowdown in the x^2 series for large spread factor and F may be due to the effects on β. When α_1 is held fixed, $\beta=2\alpha_1\alpha_n/(\alpha_1+\alpha_n)$ decreases as α_n decreases, implying that y/β increases for fixed y. If y is relatively large to begin with, then the factor $G(n+2k;y/\beta)$ in (5) decreases more slowly with k, so a larger N is required for convergence.

The convergence behavior of the x^2 series does have the following desirable property not shared by either the power series or the Laguerre series. For all sets except set 5, convergence of the x^2 series is monotonically increasing due to positive c_k's. But even for set 5, where the c_k's alternate in sign but decrease quickly in absolute value toward zero, F_N never deviates from F by more than .1. Thus, the convergence of the x^2 series is less affected by extreme intermediate results.

In summary, convergence of the three algorithms is relatively poor when both F and the spread factor are high. The power series and the Laguerre series algorithms both break down under these conditions, whereas the x^2 series algorithm

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Table 4

Partial Sums of the Power Series Before Convergence[1]

N	F_N	N	F_N
1	-19.969	28	2050.241
2	78.344	29	-1195.068
3	-250.705	30	676.940
4	705.275	31	-370.253
5	-1725.121	32	198.350
6	3743.199	33	-101.586
7	-7268.411	34	52.243
8	12777.252	35	-24.523
9	-20498.397	36	12.780
10	30247.525	37	-4.883
11	-41305.339	38	3.272
12	52497.234	39	-.401
13	-62388.877	40	1.214
14	69629.252	41	.520
15	-73243.098	42	.811
16	72862.732	43	.692
17	-68747.932	44	.740
18	61691.240	45	.721
19	-52772.204	46	.728
20	43132.243	47	.725
21	-33746.481	48	.726
22	25324.977	49	.726
23	-18256.005	50	.726
24	12664.770	51	.726
25	-8463.937	52	.726
26	5459.748	53	.726
27	-3400.437		

[1]Set 6

Table 5

Error Bounds[1]

Power series

n=3, ∞ means greater than 10^{10}, .0 means less than 10^{-10}

N	Set 1	2	3	4	5	6
20	∞	$.464 \times 10^9$	.0	.0795	∞	$.959 \times 10^5$
40	∞	$.659 \times 10^7$	.0	$.117 \times 10^{-10}$	$.149 \times 10^9$	$.1615 \times 10^1$
60	∞	$.5340 \times 10^1$	.0	.0	$.195801 \times 10^3$	$.154 \times 10^{-8}$
80	∞	$.645 \times 10^{-8}$	.0	.0	$.390 \times 10^{-6}$	.0
100	∞	.0	.0	.0	.0	.0
120	∞	.0	.0	.0	.0	.0
140	$.229 \times 10^9$	.0	.0	.0	.0	.0
160	$.5643 \times 10^1$	.0	.0	.0	.0	.0
180	$.118 \times 10^{-7}$	.0	.0	.0	.0	.0
200	.0	.0	.0	.0	.0	.0

merely slows down. Specifically how the two conditions inter-
act with equations (3), (5) and (7) is not exactly known.

Error bounds

The error bounds tend to be more informative for the
power series than for the other two series. The error bounds
start out high for the power series (see the top part of Table
5), but decrease rapidly to 0 for all sets soon after F_N
is stabilized at either the correct or incorrect (sets 1, 5)
value. However, for the χ^2 series, the rather sharp drop-
off from an astronomical value to 0 (middle of Table 5) does
not occur until after N exceeds 100 for most sets, even
though F_N converges at N<50. Also, the error bounds for
the Laguerre series decrease slowly and are often greater than
1 at N=200 (bottom of Table 5), even though the obtained
F_{200} are always correct to at least two decimal places. Thus,
for the latter two series, the error bounds do not always de-
crease in the same way as the deviation of F_N from F.

Timing runs

Each of the series algorithms was run 5, 10, and 15
times at n=4 and N=120. The slope and intercept of the
function relating computation to the number of approximations
are presented in Table 6. The intercepts do not differ greatly
from 0. The slopes indicate that an approximation using the
power series algorithm is slower than that using the χ^2 or
Laguerre series algorithms, in accordance with the dominating
terms of the equation relating number of computations to n
and N ($5/2nN^2$ vs. nN^2). Note that these timing runs

Table 5 (cont.)
Error Bounds[1]

Chi-square series

N	Set					
	1	2	3	4	5	6
40	∞	∞	∞	∞	.0	∞
80	∞	∞	∞	∞	.0	∞
120	∞	$.984 \times 10^6$	∞	∞	.0	∞
160	∞	.0	∞	∞	.0	.0232
200	$.30782 \times 10^2$	.0	.0	.0	.0	.0

[1]$n=3$, ∞ means greater than 10^{10}, .0 means less than 10^{-10}

Table 5 (cont.)
Error Bounds[1]

Laguerre series[2]

N	Set					
	1	2	3	4	5	6
40	$.25945 \times 10^4$	$.11555 \times 10^1$	$.97869 \times 10^3$	$.74445 \times 10^4$	$.42631 \times 10^{-10}$	$.36282 \times 10^3$
80	$.42204 \times 10^3$	$.94082 \times 10^{-2}$	$.28526 \times 10^3$	$.22212 \times 10^4$	.0	$.37276 \times 10^2$
120	$.90793 \times 10^2$	$.10131 \times 10^{-3}$	$.10996 \times 10^3$	$.87652 \times 10^3$	.0	$.50648 \times 10^1$
160	$.21929 \times 10^2$	$.12248 \times 10^{-5}$	$.47587 \times 10^2$	$.38832 \times 10^3$	.0	.77259
200	$.56447 \times 10^1$	$.15782 \times 10^{-7}$	$.21949 \times 10^2$	$.18335 \times 10^3$	.0	.12561

[1]$n=3$, ∞ means greater than 10^{10}, .0 means less than 10^{-10}

[2]$B=1/2(\alpha_1+\alpha_3)$

Table 6

Timing Runs[1]

Method	Slope[2]	Intercept[3]
Power series	.0815	.015
Chi-square series	.0583	.003
Laguerre series[4]	.0564	.026
DLT	.0626	.006

[1]$n=4$

[2]Seconds to compute one approximation at $N=120$

[3]Intercept of the equation relating time to number of approximations

[4]$\beta=(\alpha_1+\alpha_4)/2$

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do not indicate speed of convergence. For example, the power series is slower to compute than the Laguerre series--i.e., requires more computations, but it generally converges faster.

2.6 Summary

The series algorithms have the problem that convergence is affected by characteristics of the y and α_j, and that the error bounds are not always informative. Furthermore, the Laguerre series requires a "fudge" factor β which depends on the α_j in a complicated way. The value of β used in the analyses previously discussed may not have been correct, but the substitution of values $2/3(\alpha_1+\alpha_3)$ and $.9(\alpha_1+\alpha_3)$ did not result in faster convergence for set 1.

An algorithm is now presented which circumvents all these problems. The resulting approximation of the distribution function always converges monotonically to F for large N, and the algorithm never broke down for N up to 500 nor is convergence speed affected by F or the spread factor. Error bounds have always ranged between 10^{-3} and 10^{-8} for N between 2 and 200 and always decrease with N. Finally, the algorithm is faster than the power series algorithm but slower than the χ^2 and the Laguerre series algorithms (last row of Table 6).

This algorithm involves approximating the unit step function. The computations were carefully selected so that numerically stable results were always attained. After these computations are discussed in detail, successive order differences of the approximation are presented which speed con-

vergence considerably. Error bounds for these successive order differences are also presented. Finally, convergence speed and accuracy are discussed for the same data used to test the series algorithms.

3. APPROXIMATING THE UNIT STEP FUNCTION

An alternative to the series expansion algorithms can be obtained by developing an inversion formula for the Laplace transform, which is rigorously derived in Feller (1967, Section XIII.4, Theorem 2). An alternative derivation begins with an approximation of the unit step function

$$K(t;y) = 1 \quad t \leq y$$
$$= 0 \quad t > y .$$

Our distribution can then be written as

$$F(y) = \int_o^\infty K(t;y) f(t)dt .$$

For fixed y , the sequence

$$K_N(t;y) = \sum_{k=0}^N \frac{(Nt/y)^k}{k!} e^{-Nt/y}$$

converges pointwise to $K(t;y)$ for $t \neq y$. Using K_N , one can obtain the following approximation to $F(y)$:

$$(12) \quad F_N(y) = \int K_N(t;y) f(t)dt .$$

A value for equation (12) can be obtained using derivatives of the Laplace transform

$$\phi(\lambda) = \int_o^\infty e^{-\lambda t} f(t)dt .$$

can be expressed as the following product:

$$\phi(\lambda) = \prod_{i=1}^{n} (1+2\alpha_i \lambda)^{-1/2} .$$

There seems to have been little interest in using (13) to compute F(y). One reason for this may be that (13) converges relatively slowly to F(y). It can be shown that $|F_N(y) - F(y)|$ is $O(1/N)$. In fact, F_N can be shown to have the form

(14) $$F_N(y) = F(y) + \frac{c_1(y)}{N} + \frac{c_2(y)}{N^2} + \frac{c_3(y)}{N^3} + \cdots .$$

where 1) the $c_i(y)$ do not depend on N and 2)

$$\sum_{i=1}^{\infty} |c_i| < \infty .$$

A complete proof is available for even n (Levine, personal communication), and there is no reason to suspect that the case for odd n is essentially different. Later, this representation of F_N will be used to accelerate convergence.

Another reason for the apparent lack of an algorithm may be that a calculation involving (13) requires carefully arranging the computations in order to avoid extreme intermediate results. The Derivatives of Laplace Transform (DLT) algorithm discussed below has produced stable results for N as large as 500 .

Since the kth derivative is

$$\phi^{(k)}(\lambda) = \int_{0}^{\infty} (-t)^k e^{-\lambda t} f(t)dt ,$$

one can prove that

$$\sum_{k=0}^{N} \frac{(-N/y)^k}{k!} \phi^{(k)}(N/y) = \int_{0}^{\infty} \sum_{k=0}^{N} \frac{(Nt/y)^k}{k!} e^{-Nt/y} f(t)dt ,$$

which is just $F_N(y)$. Thus, the approximation given in equation (12) is

(13) $$F_N(y) = \sum_{k=0}^{N} \frac{(-N/y)^k}{k!} \phi^{(k)} (N/y) .$$

We will substitute λ for N/y from now on.

In order to approximate the distribution of variables of form (1) using (13), one must determine the Laplace transform of such variables. It can first of all be shown that if $X = {}_i Z^2$, where Z is a standard normal variable, then the Laplace transform of X is

$$\phi_X(\lambda) = (1+2\alpha\lambda)^{-1/2} .$$

Thus, for independent, standard normal variables Z_i, the Laplace transform of

$$\sum_{i=1}^{n} \alpha_i Z_i^2$$

3.1 DLT algorithm

The present algorithm calculates the terms in (13) by recursively evaluating $(-\lambda)^k/k!$ times the derivatives of successive products

$$\phi_m^*(\lambda) = \prod_{i=1}^{m} \phi_i(\lambda) ,$$

where

$$\phi_i(\lambda) = (1+2\alpha_i\lambda)^{-1/2} .$$

First, the values of $(-\lambda)^k/k! \ \phi_1^{(k)}(\lambda)$ are obtained at $i=N/y$ for $k=0,1,...N$ using the recursive formula

(15) $$\frac{(-\lambda)^k}{k!} \phi_1^{(k)} = \left(\frac{2k-1}{k}\right) \left(\frac{\alpha_1\lambda}{1+2\alpha_1\lambda}\right) \left[\frac{(-\lambda)^{k-1}}{(k-1)!} \phi_1^{(k-1)}\right] .$$

Then the values of $(-\lambda)^k/k!$ times the kth derivative of the product $\phi_1(\lambda)\phi_2(\lambda)$ are obtained for $k=0,1,2,...,N$, etc.

In general, the values of

$$\frac{(-\lambda)^k}{k!} \frac{d^k}{d\lambda^k} \phi_m^*$$

are obtained from the stored values involving derivatives of ϕ_{m-1}^* by the following application of Leibniz' formula:

(16) $$\frac{(-\lambda)^k}{k!} \frac{d^k}{d\lambda^k} \phi_m^* = \frac{(-\lambda)^k}{k!} \sum_{j=0}^{k} \binom{k}{j} \left(\frac{d^j}{d\lambda^j} \phi_{m-1}^*\right) \phi_m^{(k-j)} .$$

The calculation of the terms in (16) requires the following computational trick. First, $\phi_m^* = \phi_{m-1}^*\phi_m$ is

calculated and stored as a value ψ_0. Next,

$$(-\lambda) \left(\frac{d}{d\lambda} \phi_m^*\right) = (-\lambda) \left[\left(\frac{d}{d\lambda} \phi_{m-1}^*\right) \phi_m + \phi_{m-1}^* \phi_m'\right]$$

is calculated by 1) multiplying the stored value of $(-\lambda)\left(\frac{d}{d\lambda}\phi_{m-1}^*\right)$ by ϕ_m and storing the result in ψ_1 ; 2) replacing the stored ψ_0 by

$$(-\lambda)\phi_{m-1}^* \phi_m' = (-\lambda) \phi_{m-1}^* \left(\frac{-\alpha_m}{1+2\alpha_m\lambda}\right) \phi_m = \left(\frac{\alpha_m\lambda}{1+2\alpha_m\lambda}\right) \psi_0 ;$$

and 3) adding ψ_0 to ψ_1. Next,

$$\frac{(-\lambda)^2}{2} \left(\frac{d^2}{d\lambda^2} \phi_m^*\right) = \frac{(-\lambda)^2}{2} \left[\left(\frac{d^2}{d\lambda^2} \phi_{m-1}^*\right) \phi_m + 2\left(\frac{d}{d\lambda} \phi_{m-1}^*\right) \phi_m' + \phi_{m-1}^* \phi_m''\right]$$

is obtained by the following steps:

$$\psi_2 = \left[\frac{(-\lambda)^2}{2} \frac{d^2}{d\lambda^2} \phi_{m-1}^*\right]\phi_m$$

$$\psi_1 = \frac{(-\lambda)^2}{2} \left[2\left(\frac{d}{d\lambda} \phi_{m-1}^*\right) \phi_m'\right] = \left(\frac{2\alpha_m\lambda}{1+2\alpha_m\lambda}\right)\psi_1$$

$$\psi_0 = \frac{(-\lambda)^2}{2} \phi_{m-1}^* \phi_m'' = \frac{3}{2} \frac{\alpha_m\lambda}{1+2\alpha_m\lambda} \psi_0$$

$$\frac{(-\lambda)^2}{2} \frac{d^2}{d\lambda^2} \phi_m^* = \psi_0 + \psi_1 + \psi_2 .$$

and so on.

In general, $\frac{(-\lambda)^k}{k!} \frac{d^k}{d\lambda^k} \phi_m^*$ can be obtained recursively

and 3) one addition and two divisions to obtain

$$\frac{\alpha_1\lambda}{1+2\alpha_1\lambda} = \frac{1}{2+\frac{1}{\alpha_1\lambda}} \ .$$

Then, for $1\le k\le N$, an application of (15) requires 1) one subtraction, one multiplication, and one division to obtain $\frac{2k-1}{k}$ and 2) two multiplications of the three factors in (15) . Thus, the calculation of $(-\lambda)^k/k! \ \phi_1^{(k)}$, $k=0,1,...,N$, requires a total of $5N+9$ computations.

The calculation of terms involving the N derivatives of ϕ_m^* requires first the one-time calculation of 1) $N\alpha_m/y$, 2) ϕ_m , and 3)

$$\frac{1}{2+\frac{1}{\alpha_m\lambda}} \ ,$$

which requires nine computations as in (15) . Next, the calculation of a term involving the kth derivative of ϕ_m^* requires 1) one multiplication in (17) to obtain ψ_k ; 2) two subtractions and one division to obtain $2 - \frac{1}{k-j}$; $j=0,1,...,k-1$; 3) two multiplications in (18) to obtain each of $\psi_0,\psi_1,...,\psi_{k-1}$; and 4) k additions of the ψ_j or a total of $6k+1$ computations. Thus, the calculation of terms involving N derivatives of ϕ_m^* requires a total of $3N^2 + 4N + 10$ computations, which includes the initial multiplication in $\phi_{m-1}^* \ \phi_m$.

from the ψ_j terms in (16) for $\frac{(-k)^{k-1}}{(k-1)!} \frac{d^{k-1}}{d\lambda^{k-1}} \phi_{m-1}^*$.

First, set

(17) $\psi_k = [\frac{(-\lambda)^k}{k!} \frac{d^k}{d\lambda^k} \phi_{m-1}^*] \phi_m$.

where the first factor has been previously computed and stored. Next, replace ψ_j by

$$\psi_j = \binom{k}{j} \frac{(-\lambda)^k}{k!} (\frac{d^j}{d\lambda^j} \phi_{m-1}^*)\phi_m^{(k-j)}$$

$$= \binom{k}{j} \frac{(-\lambda)^k}{k!} (\frac{d^j}{d\lambda^j} \phi_{m-1}^*) [2(k-j)-1] (\frac{-\alpha_m}{1+2\alpha_m\lambda}) \phi_m^{(k-j-1)}$$

(18) $$= (2 - \frac{1}{k-j}) \frac{\lambda\alpha_m}{1+2\alpha_m\lambda} \binom{k-1}{j} [\frac{(-\lambda)^{k-1}}{(k-1)!} \frac{d^j}{d\lambda^j} \phi_{m-1}^*] \phi_m^{(k-j-1)}$$

$$= (2 - \frac{1}{k-j}) \frac{\lambda\alpha_m}{1+2\alpha_m}) \psi_j$$

for $j=0,1,2,...,k-1$. Finally, add the ψ_j .

The amount of storage required in the DLT algorithm is $2(N+1)$ cells - $N+1$ for terms involving the derivatives of ϕ_m^* and $N+1$ for the ψ_j .

The required number of computations in the DLT algorithm can be broken down into the following. The terms involving the N derivatives of ϕ_1 [obtained from (15)] require first the one-time only computations of 1) one multiplication and one division to obtain $\lambda_1=N\alpha_1/y$; 2) one addition, one multiplication, one division, and one square root calculation to obtain $\phi_1(\lambda)$;

Thus, 5N+9 computations are required to obtain terms involving the N derivatives of ϕ_1 ; $(n-1)(3N^2 + 4N + 10)$ computations are required for terms involving the N derivatives of ϕ_m^*, $m=2,...,n$; and N further additions are required in applying equation (13) . So the approximation $F_N(y)$ requires $10n + 3(n-1)N^2 + (4n+2)N - 1$ computations. The dominating term, $3(n-1)N^2$, is larger than that for the χ^2 series and Laguerre series, but smaller than that for the power series.

As was mentioned previously, F_N converges slowly. However, the representation (14) of F_N as a series in 1/N can be used to accelerate convergence and obtain error bounds.

3.2 1st order differences

Manipulation of (14) shows that the first order difference

$$D_N = NF_N - (N-1)F_{N-1}$$

has the expansion

$$D_N = F + \left(\frac{1}{N} - \frac{1}{N-1}\right)c_2 + \left(\frac{1}{N^2} - \frac{1}{(N-1)^2}\right)c_3 + \cdots .$$

For N sufficiently large, the terms after the second are negligible. Since $\left(\frac{1}{N} - \frac{1}{N-1}\right)c_2$ is monotone in N , D_N will be eventually monotone. Furthermore, since the c_1 term above cancelled out, D_N-F is $O(1/N^2)$, so D_N con-

verges much faster than F_N .

An error bound is computed for D_N as follows. The difference

$$D_N^* = (N+1)D_{N+1} - ND_N$$

also converges monotonically to F , but in opposite direction from D_N . Basically,

$$D_N^* = F + \frac{c_2}{N(N-1)} + \cdots ,$$

so the c_2 term of D_N^* is opposite in sign from the c_2 term of D_N . Furthermore, the midpoint $(D_N+D_N^*)/2$ is $F+O(1/N^3)$ (the c_2 terms cancel). Thus, an error bound is $|D_N-D_N^*|/2$.

3.3 2nd order differences

The quantity

$$E_N = \frac{N}{2} D_N - \frac{N-2}{2} D_{N-1}$$

converges in $1/N^3$, since

$$E_N = F + \frac{c_3}{N(N-1)(N-2)} + \cdots .$$

(in fact, the midpoint $(D_N+D_N^*)/2$ is equal to E_{N+1}) . Also, the quantity $(2E_N+E_N^*)/3$ converges in $1/N^4$, where

$$E_N^* = (N+1)E_{N+1} - NE_N$$

converges monotonically in the opposite direction from E_N ,

Table 7

	F_{200} Determined by DLT Methods[1]		
		Approximation	
Set	Original DLT	1st order difference	2nd order difference
1	.9633128	.9364196	.9364345
2	.97435573	.97458867	.97459031
3	.04984353	.04955660	.04955647
4	.20313927	.20233819	.20233724
5	.99999642	99999745	.99999735
6	.7260912	.72613241	.72613215

[1] n=3

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so an error bound for E_N is

$$|E_N - \frac{2E_N + E_N^*}{3}| = |\frac{E_N - E_N^*}{3}| .$$

3.4 3rd order differences

A similar argument can be used to show that 1)

$$G_N = \frac{N}{3}E_N - \frac{N-3}{3}E_{N-1}$$

converges to F monotonically and in fact equals

$(2E_{N-1} + E_{N-1}^*)/3$; 2) $G_N - F$ is $O(1/N^4)$; 3)

$$G_N^* = (N+1)G_{N+1} - NG_N$$

converges monotonically in the opposite direction; 4) the

quantity $(3G_N + G_N^*)/4$ is $F + O(1/N^5)$; and 5) $|G_N - G_N^*|/4$

is an error bound for G_N .

3.5 Testing the algorithms

Table 7 shows the values of F_{200} obtained by the DLT algorithm and the 1st and 2nd order differences. The 2nd order differences have all converged to the correct values at 5 decimal places by N=2C0 , and the 1st order differences have converged for all sets except set 5 , where F_{200} is correct at only 4 decimal places. However, the DLT approximation is correct at only 2 decimal places for sets 2, 4 and 6 ; three decimal places for sets 1 and 3 ; and fjve places for set 5 . Thus, higher order differences are more likely to have converged by N=200 .

Table 8

N Required For Convergence

Set	Approximation		
	1st order difference	2nd order difference	3rd order difference
1	84	22	12
2	112	24	12
3	-	44	17
4	71	12	6
5	30	26	16
6	63	17	11

Convergence is faster for higher order differences as well. Table 8 shows that the 2nd order differences have all converged by N=50, and that the 3rd order differences have converged by N=20. Figure 2 illustrates this for set 1 - the top relatively flat curve represents the 3rd order difference, below which lies the 2nd order difference, then the 1st order difference, and finally the DLT approximation, which converges the slowest.

The monotonic behavior of the convergence varies with the sets. All approximations increase monotonically toward F for sets 1 and 2 as is illustrated in Figure 2 for set 1 . However, the approximations decrease toward F for sets 3 and 4, and the DLT and 1st order difference approximation increase monotonically while the 2nd and 3rd order approximation decrease monotonically toward F for sets 5 and 6 (In fact, the 2nd order difference for set 5 first decreases, then increases toward F, illustrating the fact that convergence is montone only for large N).

An illustration of the error bound of the 1st order difference is presented in Figure 3 for set 1 . The bottom line represents D_N , the top line represents D_N^* , and the relatively flat line in the middle represents the midpoint $(D_N + D_N^*)/2$. The distance between D_N and its projection onto the middle line is seen to decrease with N . In fact, Table 9 shows that the error bound decreases with N for all six sets. Furthermore, the error bounds start out relatively low - never more than .001 .

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Figure 3

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Figure 2

The error bounds decrease more quickly with N for higher order differences. However, they become difficult to calculate due to roundoff error of the higher order differences. The original DLT approximation is accurate at only a finite number of decimal places, and the difference between NF_N and $(N-1)F_{N-1}$ becomes even less accurate with large N. Compounding these differences for higher order differences results in even a further loss of accuracy. The third order approximations, fortunately, do not break down at five decimal places for N as large as 200, but the error bounds of the 2nd and 3rd order differences, which are on the order $10^{-6} - 10^{-8}$, no longer are monotone for N>100.

The error bounds, however, are monotonically decreasing at N near the convergence criterion. Table 10 compares the error bounds of the 1st, 2nd and 3rd order differences at criterion values of N (listed in Table 8). First, the error bounds are never greater than 10^{-5}, consistent with the definition of convergence (at five decimal places). Second, for most sets, the error bound of the 3rd order difference is less than that of the 2nd order difference, which is less than the error bound of the 1st order difference, despite the fact that the convergence criterion is smallest for higher order differences.

3.6 Summary

Several results show that the DLT algorithm and its successive order differences are superior to the series expansion algorithms discussed earlier. First, convergence is always

Table 9

Error Bound On 1st Order Differences (X 1,000,000)

N	Set					
	1	2	3	4	5	6
10	453.	560.	52.2	390.	139.	200.
20	140.	152.	12.9	96.3	24.3	38.1
30	60.8	69.5	5.74	42.6	8.66	15.0
40	35.1	39.7	3.22	24.0	4.24	7.86
50	22.8	25.6	2.07	15.3	2.47	4.81
60	16.0	17.9	1.43	10.6	1.61	3.23
70	11.8	13.2	1.05	7.81	1.12	2.32
80	9.12	10.2	.807	5.98	.824	1.74
90	7.23	8.05	.636	4.72	.631	1.36
100	5.88	6.53	.516	3.82	.498	1.09
110	4.87	5.41	.427	3.16	.402	.891
120	4.10	4.55	.359	2.65	.331	.742
130	3.51	3.88	.305	2.26	.278	.628
140	3.01	3.35	.263	1.95	.236	.536
150	2.64	2.92	.230	1.70	.204	.466
160	2.33	2.56	.202	1.49	.177	.411
170	2.06	2.27	.179	1.32	.156	.360
180	1.84	2.03	.159	1.18	.136	.320
190	1.65	1.82	.143	1.06	.121	.285
200	1.50	1.65	.129	.954	.111	.262

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Table 10

Error At Convergence Criterion[1]

Set	1st order difference	2nd order difference	3rd order difference
1	$.8285 \times 10^{-5}$	$.7222 \times 10^{-5}$	$.5561 \times 10^{-5}$
2	$.5217 \times 10^{-5}$	$.4547 \times 10^{-5}$	$.3351 \times 10^{-5}$
3	$-^2$	$.2079 \times 10^{-7}$	$.1718 \times 10^{-7}$
4	$.7589 \times 10^{-5}$	$.7152 \times 10^{-5}$	$.6175 \times 10^{-5}$
5	$.8661 \times 10^{-5}$	$.2203 \times 10^{-5}$	$.2251 \times 10^{-5}$
6	$.2909 \times 10^{-5}$	$.6271 \times 10^{-5}$	$.4520 \times 10^{-5}$

[1] 5 decimal places, as indicated in Table 5

[2] Does not converge at $N = 200$, where error is $.129 \times 10^{-6}$

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monotone for large N, so fluctuations do not slow convergence or produce roundoff error. Second, 3rd order differences converge faster than the series expansions for most of the sets analyzed here. Third, convergence seems unaffected by such conditions as high spread factor or high F, unlike the series methods - in fact, the DLT algorithm has never failed for N as large as 500. Fourth, no fudge factor is required, unlike the Laguerre series, where β can be difficult to compute. Finally, the error bounds are small, whereas those for the series expansions sometimes start out astronomical and are still larger than 1 at $N=200$.

The superiority of the DLT method is shown by an extreme example in which $y=7.0$, $\alpha_1=1.0$, $\alpha_2=.001$, $\alpha_3=.000001$, and thus the spread factor is 100,000. The 2nd order difference converges at .99184 when $N=27$, with an error bound of $.3564 \times 10^{-6}$. However, the series algorithms fail miserably.

Much of the time, however, the higher order differences require more time to compute at convergence than do the series expansions. First, the DLT algorithm requires a time between that of the χ^2 series and the power series for a given N (see Table 6). Second, the DLT algorithm must be applied to, let's say, four successive values of N in order to obtain the 3rd order difference. Thus, convergence of the 3rd order difference at $N=20$ requires the number of calculations equivalent for N about 80, which is more than N required for the convergence of the χ^2 series for all sets (see Table 2).

a_k can be determined from the recursive equation

$$a_k = \frac{1}{k} \sum_{r=0}^{k-1} b_{k-r} a_r .$$

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But, despite the greater computing costs, the higher order differences seem to be more reliable and the error bounds seem to be more informative.

4. APPENDIX

This appendix discusses a method for obtaining a_k in the expansion

$$f_N(y) = \sum_{k=0}^{N} a_k h_k(y) .$$

Kotz, Johnson, and Boyd (1967) proved that a_k must satisfy the equality

$$\sum_{k=0}^{\infty} a_k t^k = \frac{\phi_f[\zeta(t)]}{\xi[\zeta(t)]}$$

for Re $\zeta(t) > C$, where ϕ_f is the Laplace transform of f and the Laplace transform of h_k satisfies

$$\phi_{h_k}(\lambda) = \xi(\lambda) [\zeta^{-1}(\lambda)]^k$$

for Re $\lambda > C$ and analytic ζ and ξ. Then, for given $h_k(y)$, the a_k can be determined as follows. If $\phi_f[\zeta(t)]/\xi[\zeta(t)]$ is obtained directly and

$$\sum_{k=1}^{\infty} \frac{b_k t^k}{k} = \log \sum_{k=0}^{\infty} a_k t^k$$

is obtained by expanding its logarithm, then, since one can differentiate both sides of the above equation to show that

$$\sum_{k=1}^{\infty} b_k t^{k-1} = (\sum_{k=1}^{\infty} k a_k t^{k-1})/(\sum_{k=1}^{\infty} a_k t^k) ,$$

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